Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:01 pm BST

PDB ID	:	1ED8
Title	:	STRUCTURE OF E. COLI ALKALINE PHOSPHATASE INHIBITED BY THE INORGANIC PHOSPHATE AT 1.75A RESOLUTION
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Deposited on	:	2000-01-27
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

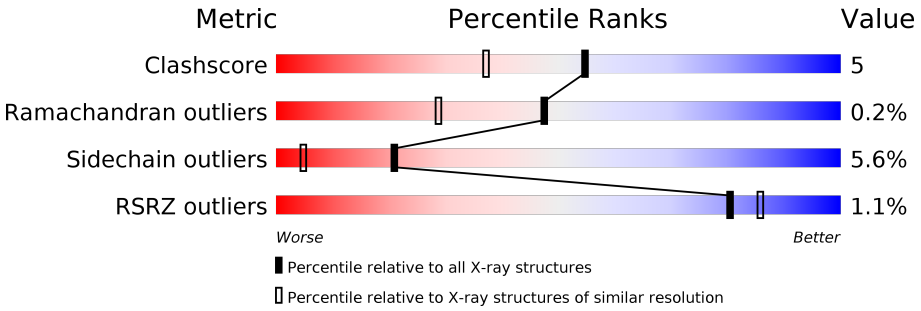
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	% 86% 12% .
1	B	449	% 82% 14% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	456	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7252 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	1	0
			3310	2045	582	671	12			
1	B	449	Total	C	N	O	S	0	1	0
			3310	2045	582	671	12			

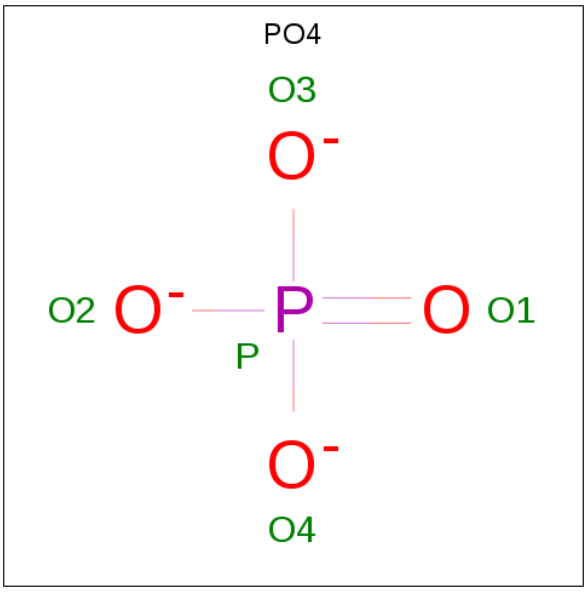
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

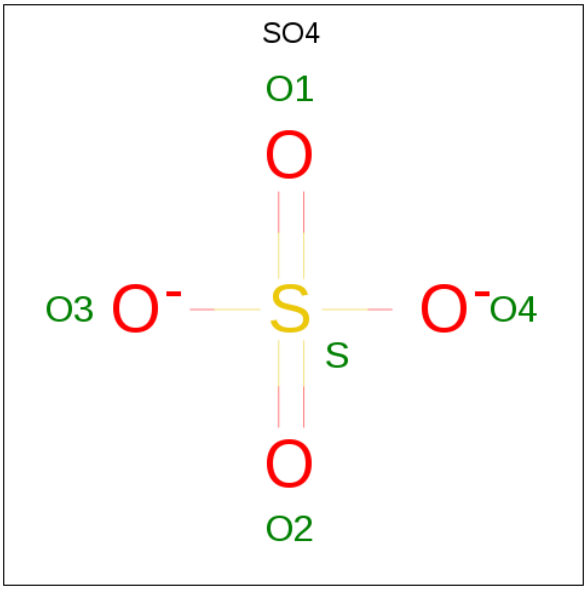
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

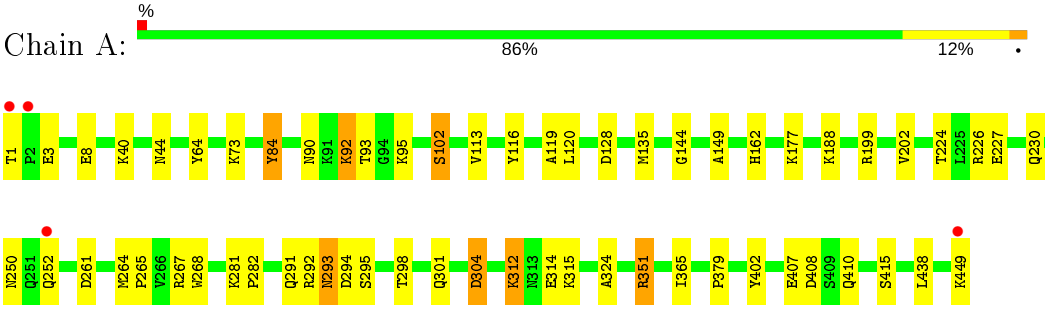
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	352	Total O 352 352	0	0
6	B	252	Total O 252 252	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

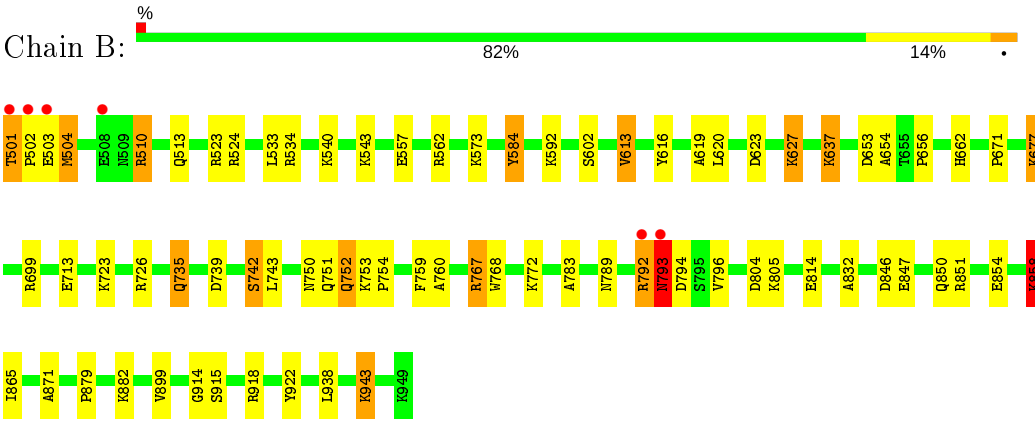
- Molecule 1: ALKALINE PHOSPHATASE

Chain A:



- Molecule 1: ALKALINE PHOSPHATASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	195.15Å 167.34Å 76.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.75 71.47 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.0 (15.00-1.75) 91.8 (71.47-1.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 1.75Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.196 , 0.228 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 78.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ZN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.86	3/3365 (0.1%)	1.19	6/4568 (0.1%)
1	B	0.82	2/3365 (0.1%)	1.17	14/4568 (0.3%)
All	All	0.84	5/6730 (0.1%)	1.18	20/9136 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	7
All	All	1	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102[A]	SER	C-N	-8.68	1.14	1.34
1	A	102[B]	SER	C-N	-8.68	1.14	1.34
1	A	415	SER	CA-CB	6.18	1.62	1.52
1	B	914	GLY	N-CA	-5.35	1.38	1.46
1	B	915	SER	CA-CB	5.20	1.60	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	A	293	ASN	N-CA-C	7.91	132.36	111.00
1	B	871	ALA	N-CA-CB	7.61	120.75	110.10
1	A	199	ARG	NE-CZ-NH2	-6.97	116.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	793	ASN	N-CA-C	6.72	129.15	111.00
1	B	562	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	64	TYR	CB-CG-CD1	6.41	124.85	121.00
1	B	584	TYR	CB-CG-CD1	6.39	124.84	121.00
1	A	84	TYR	CA-CB-CG	6.25	125.28	113.40
1	B	858	LYS	N-CA-CB	5.86	121.15	110.60
1	B	504	MET	N-CA-CB	5.65	120.76	110.60
1	B	783	ALA	N-CA-CB	5.46	117.74	110.10
1	B	943	LYS	CA-CB-CG	5.43	125.34	113.40
1	A	268	TRP	CA-CB-CG	5.39	123.93	113.70
1	B	534	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	613	VAL	CA-CB-CG1	5.22	118.73	110.90
1	B	510	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	557	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	B	524	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	534	ARG	NE-CZ-NH2	5.04	122.82	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	293	ASN	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ARG	Sidechain
1	A	351	ARG	Sidechain
1	B	510	ARG	Sidechain
1	B	699	ARG	Sidechain
1	B	726	ARG	Sidechain
1	B	767	ARG	Sidechain
1	B	792	ARG	Sidechain
1	B	851	ARG	Sidechain
1	B	918	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3310	0	3252	34	0
1	B	3310	0	3249	33	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	2	0
4	B	5	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
6	A	352	0	0	14	0
6	B	252	0	0	6	0
All	All	7252	0	6501	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602[A]:SER:OG	6:B:999:HOH:O	1.52	1.24
1:A:102[A]:SER:OG	6:A:499:HOH:O	1.60	1.17
1:A:312:LYS:HE2	6:A:1137:HOH:O	1.78	0.84
1:A:102[B]:SER:OG	4:A:456:PO4:P	2.29	0.81
1:A:298:THR:OG1	1:A:301:GLN:HG3	1.91	0.71
1:A:73:LYS:HE3	6:A:1142:HOH:O	1.90	0.70
1:A:291:GLN:HG3	6:A:1174:HOH:O	1.97	0.63
1:A:224:THR:OG1	1:A:227:GLU:HG3	1.98	0.63
1:A:379:PRO:HD2	6:A:1595:HOH:O	1.98	0.63
1:B:789:ASN:O	1:B:792:ARG:HD3	1.99	0.62
1:B:943:LYS:HE2	6:B:1419:HOH:O	2.02	0.59
1:B:654:ALA:HB3	6:B:1546:HOH:O	2.03	0.57
1:B:653:ASP:O	1:B:656:PRO:HD2	2.05	0.56
1:B:739:ASP:OD2	1:B:742:SER:OG	2.24	0.54
1:B:501:THR:O	1:B:503:GLU:N	2.40	0.54
1:A:267:ARG:HG3	6:A:1183:HOH:O	2.07	0.53
1:B:513:GLN:HG2	1:B:523:ARG:O	2.09	0.53
1:B:750:ASN:OD1	1:B:752:GLN:HG2	2.09	0.52
1:A:120:LEU:O	1:A:162:HIS:HA	2.09	0.52
1:A:95:LYS:NZ	6:A:1336:HOH:O	2.43	0.52
1:B:854:GLU:O	1:B:858:LYS:HG3	2.10	0.51
1:B:793:ASN:HB3	1:B:796:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:OD1	1:A:92:LYS:HG2	2.11	0.51
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.46	0.50
1:B:859:GLU:OE2	1:B:861:ASN:N	2.31	0.50
1:B:501:THR:HG23	1:B:502:PRO:HD2	1.94	0.50
1:A:407:GLU:HB2	6:A:1232:HOH:O	2.12	0.49
1:A:304:ASP:CG	1:A:351:ARG:HH21	2.16	0.49
1:B:793:ASN:OD1	1:B:794:ASP:N	2.45	0.49
1:B:620:LEU:O	1:B:662:HIS:HA	2.13	0.48
1:B:616:TYR:CZ	1:B:619:ALA:HB2	2.49	0.47
1:B:879:PRO:HA	1:B:899:VAL:HG21	1.96	0.47
5:A:458:SO4:O1	6:A:1465:HOH:O	2.20	0.46
1:A:92:LYS:HG2	1:A:93:THR:HG23	1.97	0.46
1:B:671:PRO:HD2	1:B:713:GLU:OE1	2.14	0.46
1:B:767:ARG:NH2	1:B:847:GLU:OE2	2.48	0.46
1:B:752:GLN:HG3	6:B:1514:HOH:O	2.15	0.46
1:A:295:SER:HA	6:A:1335:HOH:O	2.16	0.45
1:B:743:LEU:O	1:B:805:LYS:HE2	2.16	0.45
1:B:735:GLN:HG3	1:B:754:PRO:O	2.17	0.45
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.99	0.45
1:B:504:MET:O	1:B:922:TYR:OH	2.23	0.45
1:B:627:LYS:HD3	6:B:1457:HOH:O	2.16	0.45
1:B:767:ARG:HD3	1:B:768:TRP:NE1	2.32	0.44
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.99	0.43
1:A:177:LYS:O	6:A:1481:HOH:O	2.20	0.43
1:A:144:GLY:HA2	1:A:202:VAL:O	2.18	0.43
1:B:846:ASP:O	1:B:850:GLN:HG3	2.18	0.43
1:B:677:LYS:C	1:B:679:PRO:HD3	2.39	0.43
1:B:772:LYS:CE	1:B:832:ALA:O	2.67	0.43
1:A:402:TYR:HB3	1:A:410:GLN:HG3	2.01	0.43
1:A:264:MET:HB3	1:A:265:PRO:HD2	2.01	0.42
1:B:865:ILE:HD13	1:B:938:LEU:HD11	2.01	0.42
1:B:859:GLU:OE1	1:B:861:ASN:HB2	2.19	0.42
1:A:149:ALA:HB2	1:A:324:ALA:HB1	2.02	0.42
1:A:188:LYS:HE3	6:A:1306:HOH:O	2.19	0.42
1:B:759:PHE:O	1:B:760:ALA:HB2	2.20	0.41
1:A:135:MET:HE3	6:A:1565:HOH:O	2.21	0.41
1:B:623:ASP:HB2	6:B:1089:HOH:O	2.20	0.41
1:A:128:ASP:OD1	1:A:188:LYS:HE3	2.20	0.41
1:A:102[B]:SER:CB	4:A:456:PO4:P	3.09	0.41
1:A:1:THR:O	1:A:3:GLU:N	2.53	0.41
1:A:250:ASN:OD1	1:A:252:GLN:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:HG3	1:A:236:LEU:CD1	2.51	0.41
1:A:298:THR:HG1	1:A:301:GLN:HG3	1.80	0.41
1:A:188:LYS:CE	6:A:1306:HOH:O	2.69	0.40
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.52	0.40
1:B:637:LYS:HE3	1:B:751:GLN:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	448/449 (100%)	440 (98%)	7 (2%)	1 (0%)	47 29
1	B	448/449 (100%)	438 (98%)	9 (2%)	1 (0%)	47 29
All	All	896/898 (100%)	878 (98%)	16 (2%)	2 (0%)	47 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	B	793	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/340 (100%)	324 (95%)	17 (5%)	24 6
1	B	341/340 (100%)	320 (94%)	21 (6%)	18 4
All	All	682/680 (100%)	644 (94%)	38 (6%)	21 5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	40	LYS
1	A	44	ASN
1	A	84	TYR
1	A	92	LYS
1	A	113	VAL
1	A	235	GLN
1	A	236	LEU
1	A	261	ASP
1	A	292	ARG
1	A	294	ASP
1	A	304	ASP
1	A	312	LYS
1	A	314	GLU
1	A	315	LYS
1	A	408	ASP
1	A	449	LYS
1	B	501	THR
1	B	533	LEU
1	B	540	LYS
1	B	543	LYS
1	B	573	LYS
1	B	584	TYR
1	B	592	LYS
1	B	613	VAL
1	B	627	LYS
1	B	637	LYS
1	B	677	LYS
1	B	685	LYS
1	B	723	LYS
1	B	735	GLN
1	B	742	SER
1	B	752	GLN
1	B	753	LYS
1	B	804	ASP

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Mol	Chain	Res	Type
1	B	814	GLU
1	B	858	LYS
1	B	882	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	B	730	GLN
1	B	752	GLN
1	B	829	GLN
1	B	838	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	B	958	-	4,4,4	0.58	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	A	458	-	4,4,4	0.63	0	6,6,6	0.24	0
4	PO4	B	956	1,2	4,4,4	0.90	0	6,6,6	0.24	0
4	PO4	A	456	1,2	4,4,4	1.12	0	6,6,6	0.83	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	458	SO4	1	0
4	A	456	PO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	102[A]:SER	C	103:ALA	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	449/449 (100%)	-0.25	4 (0%)	84	89	9, 18, 41, 127	0
1	B	449/449 (100%)	-0.11	6 (1%)	77	83	11, 23, 53, 129	0
All	All	898/898 (100%)	-0.18	10 (1%)	80	86	9, 20, 50, 129	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	THR	15.1
1	A	1	THR	12.3
1	A	2	PRO	7.6
1	B	502	PRO	4.3
1	A	449	LYS	3.4
1	B	503	GLU	3.2
1	B	793	ASN	2.6
1	B	508	GLU	2.3
1	B	792	ARG	2.2
1	A	252	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	958	5/5	0.94	0.13	60,62,72,72	5
5	SO4	A	458	5/5	0.96	0.10	35,53,58,60	0
4	PO4	A	456	5/5	0.97	0.07	18,18,19,19	0
4	PO4	B	956	5/5	0.98	0.07	18,21,24,24	0
2	ZN	B	950	1/1	0.99	0.03	16,16,16,16	0
2	ZN	A	452	1/1	0.99	0.03	9,9,9,9	1
2	ZN	B	952	1/1	0.99	0.07	20,20,20,20	1
3	MG	A	462	1/1	0.99	0.03	9,9,9,9	1
3	MG	B	962	1/1	0.99	0.07	20,20,20,20	1
2	ZN	A	450	1/1	0.99	0.03	14,14,14,14	0
2	ZN	A	451	1/1	0.99	0.03	13,13,13,13	0
2	ZN	B	951	1/1	1.00	0.03	17,17,17,17	0

6.5 Other polymers

There are no such residues in this entry.